

Solution of the Holstein polaron anisotropy problem

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We study Holstein polarons in three-dimensional anisotropic materials. Using a variational exact diagonalization technique we provide highly accurate results for the polaron mass and polaron radius. With these data we discuss the differences between polaron formation in dimension one and three, and at small and large phonon frequency. Varying the anisotropy we demonstrate how a polaron evolves from a one-dimensional to a three-dimensional quasiparticle. We thereby resolve the issue of polaron stability in quasi-one-dimensional substances and clarify to what extent such polarons can be described as one-dimensional objects. We finally show that even the local Holstein interaction leads to an enhancement of anisotropy in charge carrier motion.

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I. INTRODUCTION

In materials with a local coupling of the charge carriers to optical phonons a tendency towards formation of polarons prevails. How polarons form, and which properties they possess, has been intensively studied using the Holstein model (for a recent review see Ref. 1). Much work was devoted to the question how polaronic properties depend on dimensionality. For zero phonon frequency polaron formation is known to be fundamentally different in dimension one (1D) and three (3D): While in 1D a polaron exists for all coupling strengths, in 3D a transition from a free electron to a self-trapped polaron occurs at a finite coupling strength². While the 3D polaron is small, in 1D large polarons with a size of many lattice constants may exist³. This qualitative difference is peculiar to the static case. At finite phonon frequencies no strict self-trapping transition occurs⁴. Instead a smooth crossover from a light electron to a heavy small polaron takes place with increasing coupling strength. Only in the adiabatic regime of small phonon frequencies, large and heavy polarons can be found in 1D⁵. In the anti-adiabatic limit of large phonon frequencies polaron properties do not depend on dimension. For intermediate phonon frequencies numerical studies⁶ reveal that in 3D polarons form as smaller and heavier quasiparticles if compared to the 1D case, but a clear distinction as for zero phonon frequency or in the adiabatic regime is not found.

Most work on the Holstein polaron problem was performed for 1D or isotropic systems. Much less attention is paid to the question how polaron properties in anisotropic materials, e.g. molecular crystals⁷, interpolate between the 1D and 3D behaviour. In particular, even polarons in quasi-1D systems, such as in organic conductors like the Bechgaard salts, are frequently described by the 1D Holstein model, neglecting the possibility of electron motion transverse to a quasi-1D chain. For zero phonon frequency Emin showed⁸ that already tiny electronic transfer integrals perpendicular to the chain

suffice to destabilize a large 1D polaron, resulting in a free electron as in 3D below the self-trapping transition. This result not only puts the existence of large (adiabatic) polarons in real materials in doubt, but also raises the question to which degree polarons in quasi-1D systems can be described as true 1D polarons. In the present work we study to which extent the scenario described for zero phonon frequency translates to finite phonon frequencies beyond the extreme adiabatic regime.

II. ANISOTROPIC POLARON MODEL

To address this fundamental question, we consider the 3D Holstein polaron model with anisotropic hopping

$$H = - \sum_{i=x,y,z} t_i \sum_{\mathbf{n}} \left(c_{\mathbf{n}+\mathbf{e}_i}^\dagger c_{\mathbf{n}} + c_{\mathbf{n}}^\dagger c_{\mathbf{n}+\mathbf{e}_i} \right) - \sqrt{\varepsilon_p \omega_0} \sum_{\mathbf{n}} (b_{\mathbf{n}}^\dagger + b_{\mathbf{n}}) c_{\mathbf{n}}^\dagger c_{\mathbf{n}} + \omega_0 \sum_{\mathbf{n}} b_{\mathbf{n}}^\dagger b_{\mathbf{n}}. \quad (1)$$

Here \mathbf{n} labels the sites of a cubic lattice, and \mathbf{e}_i for $i = x, y, z$ denotes the unit lattice vector in the respective direction. ω_0 is the phonon frequency, and ε_p the electron-phonon coupling strength. For the electron transfer integrals, we set $t_x = t_{\parallel}$, $t_y = t_z = t_{\perp}$. As t_{\perp}/t_{\parallel} grows, the system described by the Hamiltonian (1) evolves from a 1D ($t_{\perp}/t_{\parallel} = 0$) to an isotropic 3D system ($t_{\perp}/t_{\parallel} = 1$). For intermediate values of t_{\perp}/t_{\parallel} , the system is anisotropic but symmetric with respect to the y, z -direction, i.e., the chains in a quasi-1D system ($t_{\perp}/t_{\parallel} \ll 1$) are oriented along the x -direction.

In addition to Ref. 8, the anisotropic Holstein model (1) has been studied in Refs. 9,10 in certain limiting cases, or using approximate variational techniques. At present, no conclusive answers for small-to-intermediate phonon frequency have been given. In this work, we present accurate results for the infinite system using the variational exact diagonalization technique developed in Ref. 11. The error of all results is generally

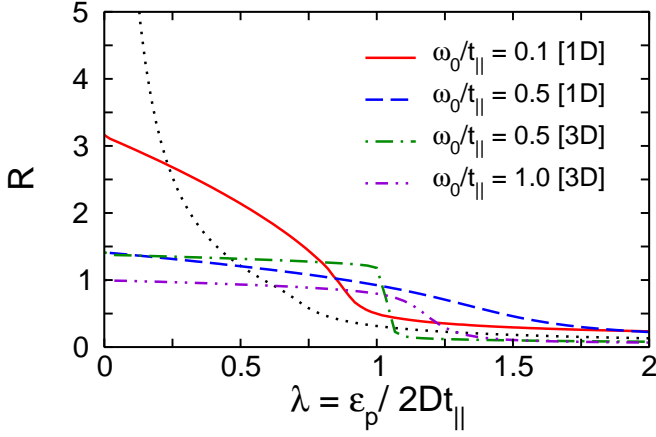


FIG. 1: (Color online) Polaron radius R as a function of coupling λ , for dimension $D = 1$ ($t_{\perp} = 0$) and $D = 3$ (isotropic case $t_{\parallel} = t_{\perp}$). The dotted curve gives the radius for $\omega_0 = 0$ and 1D, which is defined according to Eq. (2) using the electron density $|\psi(\mathbf{r})|^2$ instead of the correlation function $\chi(\mathbf{r})$.

much less than 1%, and about 1% for the polaron radius in the crossover regime at small ω_0 in 3D. Our presentation concentrates on small-to-intermediate phonon frequencies $\omega_0/t_{\parallel} = 0.1 \dots 2.0$. We justify this choice in the next paragraphs.

III. NUMERICAL RESULTS AND DISCUSSION

A. 1D and 3D cases

The destabilization of a polaron at small t_{\perp}/t_{\parallel} occurs only if the polaron is large.⁸ We therefore begin our discussion with the basic question in what cases large polarons exist at finite phonon frequencies. Using the electron-phonon correlation function $\chi(\mathbf{r}) = \sum_{\mathbf{n}} \langle \psi_0 | (b_{\mathbf{n}+\mathbf{r}}^{\dagger} + b_{\mathbf{n}+\mathbf{r}}) c_{\mathbf{n}}^{\dagger} c_{\mathbf{n}} | \psi_0 \rangle$, the polaron radius, which measures the extension of the phonon cloud surrounding the electron, is defined as

$$R_{\parallel} = \left[\frac{\sum_{\mathbf{r}} (r_x)^2 \chi(\mathbf{r})}{2 \sum_{\mathbf{r}} \chi(\mathbf{r})} \right]^{1/2}, \quad (2)$$

and similarly for R_{\perp} with r_x replaced by r_y or r_z . Note that for the Holstein model, $\sum_{\mathbf{r}} \chi(\mathbf{r}) = 2\sqrt{\epsilon_p/\omega_0}$.

How the distinctive features of polaron formation found for zero phonon frequency persist at small ω_0/t_{\parallel} is manifest in a comparison of the 1D ($t_{\perp}/t_{\parallel} = 0$) and 3D ($t_{\perp}/t_{\parallel} = 1$) curves for $R = R_{\parallel} = R_{\perp}$ in Fig. 1, given as a function of $\lambda = \epsilon_p/2Dt_{\parallel}$. The step decrease of R in the vicinity of $\lambda = 1$ for 3D, $\omega_0/t = 0.5$ is a precursor of the self-trapping transition for $\omega_0 = 0$, which takes place at $\lambda_c^{3D} \approx 0.90$. In 1D the polaron radius decreases steadily with λ , and no crossover region can be identified. Although the latter behaviour is reminiscent of the

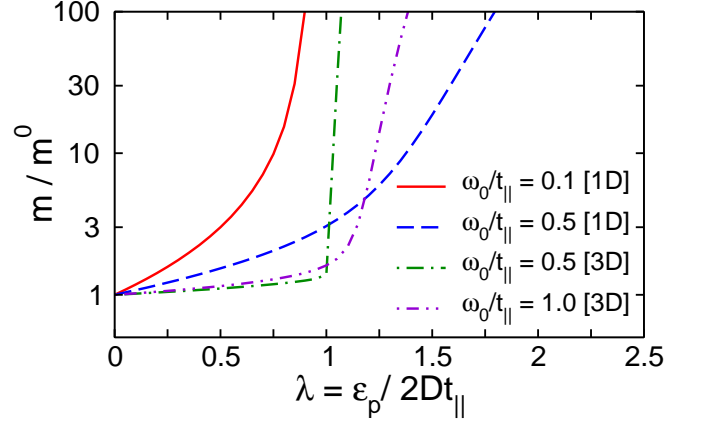


FIG. 2: (Color online) Polaron mass m as a function of coupling λ , for the parameters as in the previous figure.

1D large-to-small polaron crossover at $\omega_0 = 0$, we observe that even for small phonon frequency $\omega_0/t_{\parallel} = 0.1$ no large polaron is found. In Ref. 13 it was shown that, independent of dimension, for weak coupling the polaron radius approaches

$$\lim_{\epsilon_p \rightarrow 0} R_{\parallel} = \sqrt{t_{\parallel}/\omega_0} \quad (3)$$

(compare the 1D and 3D curve for $\omega_0/t_{\parallel} = 0.5$ in Fig. 1). The polaron radius is bounded by that limiting value, e.g., for $\omega_0/t_{\parallel} = 0.1$, at most $R_{\parallel} < 3.2$. To obtain a large polaron of radius greater than 5 or 10, ω_0/t_{\parallel} must be less than 0.01 to 0.04 for weak coupling ϵ_p/ω_0 , $\lambda \ll 1$. Furthermore the polaron shrinks rapidly with increasing coupling. Even for $\omega_0 = 0$ a coupling of, say, $\lambda \gtrsim 0.25$ leads to a polaron radius of only $R \lesssim 2$. The condition on the phonon frequency this becomes even more restrictive if we ask for large polarons with substantial mass, in contrast to the light large polarons at weak coupling.

The polaron mass, which is probably the most important quantity to characterize a polaron, is defined as

$$m_i^{-1} = \left. \frac{\partial^2 E(\mathbf{k})}{\partial k_i^2} \right|_{\mathbf{k}=0}, \quad (4)$$

where $E(\mathbf{k})$ is the groundstate energy at momentum \mathbf{k} . We set $m_{\parallel} = m_x$, and $m_{\perp} = m_y = m_z$. In the absence of electron-phonon coupling ($\epsilon_p = 0$), the masses are given by $m_{\parallel}^0 = 1/2t_{\parallel}$, $m_{\perp}^0 = 1/2t_{\perp}$. At $\omega_0 = 0$ the (3D) transition from a free electron to a self-trapped polaron coincides with a jump of m_i from $m_i = m_i^0$ (below the transition) to $m_i = \infty$ (above the transition). For finite ω_0 , m depends analytically on the coupling strength ϵ_p^4 .

In Fig. 2 we show the polaron mass $m = m_{\parallel}$ as a function of the coupling strength $\lambda = \epsilon_p/2Dt_{\parallel}$, for different ω_0 in dimension $D = 1, 3$. Remember that the data for m correspond to the exact numerical solution of the Holstein model. As for the radius the distinctive differences of polaron formation in 1D and 3D are manifest in a comparison of the corresponding curves for $\omega_0/t_{\parallel} = 0.5$.

While in 1D the polaron mass increases steadily with λ , a steep increase of m_{\parallel} occurs in the vicinity of λ_c^{3D} for 3D. One can therefore locate, for small phonon frequency $\omega_0/t_{\parallel} \lesssim 1$ in 3D, the crossover from a light particle to a heavy polaron in the region $\lambda \simeq 1$, while in 1D no crossover region can be identified. The differences between 1D and 3D vanish for larger phonon frequencies $\omega_0/t_{\parallel} \gtrsim 1$ (not shown here), where the mass indicates the continuous evolution from a light to a heavy polaron with increasing λ . In the anti-adiabatic regime $\omega_0/t_{\parallel} \gg 1$, the relation $m_i/m_i^0 = \exp(g^2)$ with $g^2 = \varepsilon_p/\omega_0$ holds independent of dimension.

The behaviour of the 1D polaron mass for small phonon frequency is reminiscent of the large-to-small polaron crossover in the $\omega_0 = 0$ -limit. However, for $\omega_0 = 0$ the mass of the 1D polaron is strictly infinite for any coupling strength in 1D. The $\omega_0 = 0$ -result therefore does not provide a quantitative prediction for the polaron mass at any finite phonon frequency. Owing to that restriction, it is also not sufficient to establish the existence of large polarons with substantial mass renormalization even for the adiabatic case $\omega_0/t_{\parallel} \ll 1$. Instead we see in Fig. 2, that even for a small phonon frequency $\omega_0/t_{\parallel} = 0.1$ the mass of the 1D polaron is still close to unity for those coupling strengths $\lambda \lesssim 0.25$, for which a large polaron is found for sufficiently small ω_0/t_{\parallel} . To obtain polarons with large mass and large radius therefore requires small coupling strengths $\lambda \ll 1$ (to allow for a large radius) and even smaller phonon frequencies $\omega_0/t_{\parallel} \ll \lambda$ (to allow for a large mass). Consequently, such heavy adiabatic large polarons may exist only at extremely small phonon frequencies $\omega_0/t_{\parallel} \lesssim 0.01$. We note that (i) in general no large-to-small polaron crossover occurs even at small phonon frequencies in 1D, (ii) the adiabatic regime of large (heavy) polarons occupies only the very narrow parameter region of tiny phonon frequencies, thus (iii) the destabilization of large quasi-1D polarons at small t_{\perp}/t_{\parallel} Emin obtained for $\omega_0 = 0$ can be expected to be relevant only in that narrow region. Qualitatively, we expect strong deviations from the findings for $\omega_0 = 0$ even for small-to-intermediate phonon frequencies beyond the extreme adiabatic regime.

B. Spatial anisotropic case

Let us now begin with the quantitative discussion of the anisotropic case. Since in the extreme adiabatic regime of large (heavy) polarons the question of polaron properties in anisotropic materials was already settled by Emin⁸ we exclude this narrow region from our further consideration. Instead we concentrate on the broader regime of small-to-intermediate phonon frequencies.

Obviously, the polaron radius does not indicate per se to which degree the polaron ceases to be a true 1D particle for small t_{\perp}/t_{\parallel} . We may instead use the ratio R_{\perp}/R_{\parallel} (see Fig. 3), which we interpret as a measure of the “one-dimensionality” of the polaron: For $R_{\perp}/R_{\parallel} = 0$

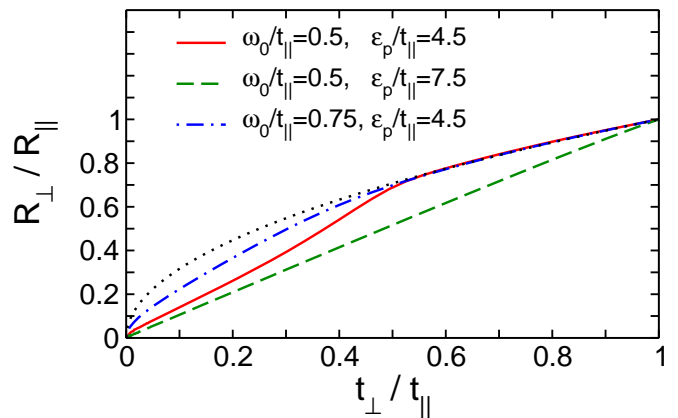


FIG. 3: (Color online) Ratio R_{\perp}/R_{\parallel} of polaron radii as a function of anisotropy t_{\perp}/t_{\parallel} , for ω_0/t_{\parallel} and $\varepsilon_p/t_{\parallel}$ as indicated. Here the dotted curve gives the weak-coupling result $R_{\perp}/R_{\parallel} = \sqrt{t_{\perp}/t_{\parallel}}$.

($R_{\perp}/R_{\parallel} = 1$), the polaron is a fully 1D (isotropic 3D) object. We see that already for small t_{\perp}/t_{\parallel} the ratio R_{\perp}/R_{\parallel} deviates significantly from zero, but R_{\perp}/R_{\parallel} is a continuous function of t_{\perp}/t_{\parallel} in contrast to the behaviour in the $\omega_0 = 0$ -limit. For weak coupling, we recover $R_{\perp}/R_{\parallel} = \sqrt{t_{\perp}/t_{\parallel}}$, as can be derived by perturbation theory¹³. For strong coupling, the asymptotic behaviour $R_{\perp}/R_{\parallel} = t_{\perp}/t_{\parallel}$ is approached. For intermediate coupling ($\varepsilon_p/t_{\parallel} = 4.5$ in the figure) we observe how the curve interpolates between the strong-coupling straight line at smaller t_{\perp}/t_{\parallel} and the weak-coupling square root at larger t_{\perp}/t_{\parallel} . To understand this observation, we shall now use the polaron mass to further clarify how the polaron properties change with t_{\perp}/t_{\parallel} .

In Fig. 4 we show the polaron mass m_{\parallel} as a function of the coupling strength $\lambda = \varepsilon_p/2(t_{\parallel} + 2t_{\perp})$, for different ω_0 and anisotropy t_{\perp}/t_{\parallel} . We see that the curves for intermediate values of t_{\perp}/t_{\parallel} smoothly interpolate between the 1D and 3D case. In contrast to the $\omega_0 = 0$ -limit a sudden transition from 1D to 3D behaviour at small t_{\perp}/t_{\parallel} is missing. Nevertheless, for $\omega_0/t_{\parallel} = 0.5$ and $\lambda > 1$, the mass m_{\parallel} increases by a huge factor if t_{\perp}/t_{\parallel} grows from zero to one. Note that this scenario is opposite to polaron destabilization in the $\omega_0 = 0$ -limit, where a large polaron evolves into a free electron at weaker coupling $\lambda < 1$ (cf. $R(\omega_0 = 0)$ in Fig. 1).

In Fig. 5 we show m_{\parallel} as a function of t_{\perp}/t_{\parallel} for fixed ε_p . Generally, the polaron mass m_{\parallel} decreases with increasing t_{\perp} . For larger phonon frequencies, m_{\parallel} depends only weakly on t_{\perp}/t_{\parallel} , in agreement with our considerations above. For small phonon frequency ($\omega_0/t_{\parallel} = 0.5$), we see how a heavy 1D polaron with $m_{\parallel}/m_{\parallel}^0 \gg 1$ evolves into a light 3D particle with $m_{\parallel}/m_{\parallel}^0 \approx 1$ as t_{\perp}/t_{\parallel} grows from zero to one. This behaviour occurs if the coupling is sufficiently large to create a heavy polaron in 1D (i.e. $\varepsilon_p/2t_{\parallel} \gg 1$) but below the heavy polaron crossover region $\lambda \simeq 1$ in 3D seen in the left panel in Fig. 4 (i.e.

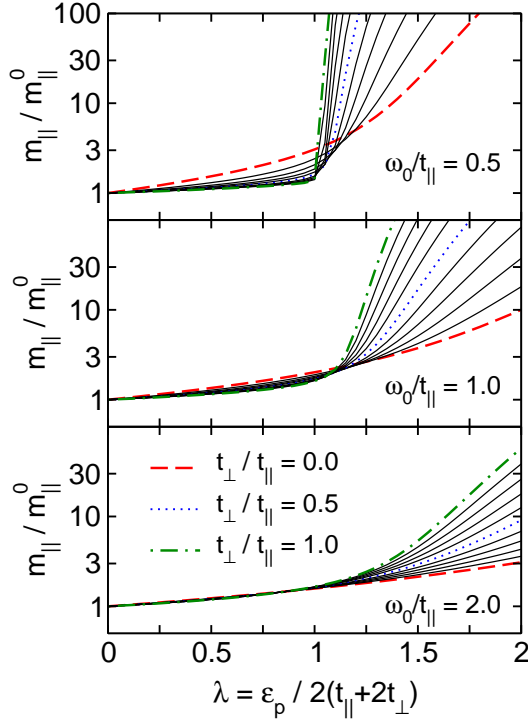


FIG. 4: (Color online) Polaron mass m_{\parallel} for different anisotropy t_{\perp}/t_{\parallel} , and phonon frequencies ω_0 as indicated. In each panel, eleven curves for $t_{\perp}/t_{\parallel} = 0.0 \dots 1.0$ in steps of 0.1 are shown. Note that for fixed $\lambda = \varepsilon_p/2(t_{\parallel} + 2t_{\perp})$ the coupling ε_p depends on t_{\perp} .

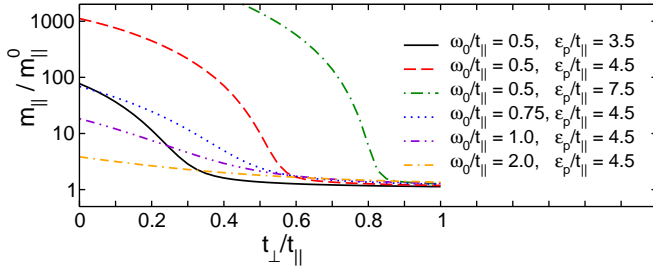


FIG. 5: (Color online) Polaron mass m_{\parallel} as a function of anisotropy t_{\perp}/t_{\parallel} , for ω_0/t_{\parallel} and $\varepsilon_p/t_{\parallel}$ as indicated.

$\varepsilon_p/6t_{\parallel} < 1$). Exactly then the ratio R_{\perp}/R_{\parallel} interpolates between the strong- and weak-coupling curve (cf. Fig. 3). Based on this condition a rough estimate for the t_{\perp}/t_{\parallel} value when the particle finally becomes light (i.e. $m_{\parallel}/m_{\parallel}^0 \approx 1$) is provided by the comparison of coupling energy to kinetic energy, yielding $\varepsilon_p/2(t_{\parallel} + 2t_{\perp}) \gtrsim 1$ or $t_{\perp}/t_{\parallel} \gtrsim (\varepsilon_p/t_{\parallel} - 2)/4$, e.g. $t_{\perp}/t_{\parallel} \gtrsim 0.5$ for $\varepsilon_p/t_{\parallel} = 4.5$. This estimate does essentially not depend on phonon frequency. Especially, our findings persist also for $\omega_0/t_{\parallel} < 0.5$.

The observed evolution from a heavy to a light particle at small-to-intermediate phonon frequency is the equivalent of polaron destabilization in the $\omega_0 = 0$ -limit. We however note significant differences to the $\omega_0 = 0$ sce-

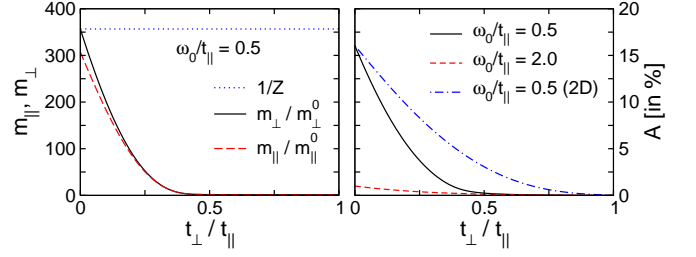


FIG. 6: (Color online) m_{\parallel} , m_{\perp} and mass renormalization anisotropy A as a function of t_{\perp}/t_{\parallel} , for $\varepsilon_p/t_{\parallel} = 4.0$. Left panel: For $t_{\perp}/t_{\parallel} \rightarrow 0$, the renormalization m_{\perp}/m_{\perp}^0 is given by the inverse quasiparticle weight $1/Z$ (dotted line). Right panel: In addition, A is shown for a 2D system.

nario. First, it requires coupling strengths for which the 1D polaron is not large. If the coupling is weak enough to allow for a large 1D polaron, no significant change of the polaron mass can occur on increasing t_{\perp}/t_{\parallel} since the 1D mass is already of the order $m_{\parallel}/m_{\parallel}^0 \simeq 1$. Recall that we exclude the extreme adiabatic regime, where this statement may be violated for extremely small phonon frequencies, from our considerations. Second, in contrast to the behaviour at zero phonon frequency, the change in m_{\parallel} takes place in a large range of t_{\perp}/t_{\parallel} , and does not occur as a rapid crossover in the vicinity of a small t_{\perp}/t_{\parallel} -value. These differences clearly show that the concept of polaron destabilization in quasi-1D systems is only of restricted relevance at finite phonon frequencies. This is a consequence of the fact that the arguments for $\omega_0 = 0$ rely on the existence of large polarons. As discussed before, those fail to exist even at small phonon frequencies $\omega_0/t_{\parallel} \lesssim 0.1$.

A repeated question raised for quasi-1D systems is whether a local or isotropic electron-phonon interaction can enhance the anisotropy in the electronic transfer integrals, leading to $m_{\perp}/m_{\parallel} > (t_{\perp}/t_{\parallel})^{-1}$. Large anisotropies in polaron mobility that exceed the estimates from, e.g., band structure calculations by several orders of magnitude can be explained if acoustic phonons are taken into account¹². It is common belief that a similar mechanism is absent in the Holstein model due to the purely local interaction with isotropic optical phonons.

As a measure for the anisotropy of mass renormalization, we define

$$A = \frac{m_{\perp}/m_{\perp}^0 - m_{\parallel}/m_{\parallel}^0}{m_{\parallel}/m_{\parallel}^0}, \quad (5)$$

or equivalently $m_{\perp}/m_{\parallel} = (1 + A)m_{\perp}^0/m_{\parallel}^0$. In the anti-adiabatic strong-coupling limit, with $m_i/m_i^0 = \exp(g^2)$, the mass renormalization is isotropic ($A = 0$), but for smaller phonon frequency $A \neq 0$ is possible. An enhancement of anisotropy corresponds to $A > 0$.

In Fig. 6 we show m_{\parallel} , m_{\perp} and the ratio A for three choices of parameters. We see that generally $m_{\perp} > m_{\parallel}$, and A is maximal for $t_{\perp} = 0$, while of course $A = 0$

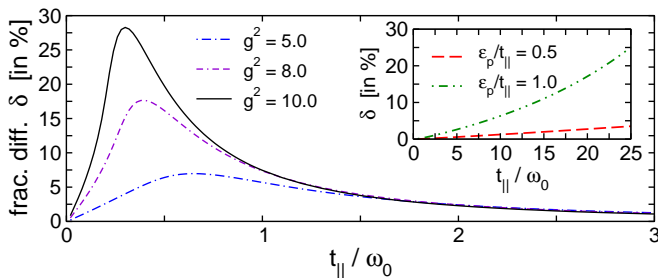


FIG. 7: (Color online) Fractional difference δ between $m_{||}/m_{||}^0$ and Z as a function of $\omega_0/t_{||}$, in 1D with $t_{\perp} = 0$, for fixed $g^2 = \varepsilon_p/\omega_0$, or fixed $\varepsilon_p/t_{||}$ in the inset.

for $t_{\perp}/t_{||} = 1$. Evidently, A is largest for small phonon frequency and large coupling, when deviations from the anti-adiabatic limit with $A = 0$ are most significant.

From first order perturbation theory in t_{\perp} we conclude that $A \rightarrow \delta$ for $t_{\perp} \rightarrow 0$, where

$$\delta = \frac{(m_{||}^0/m_{||})_{t_{\perp}=0} - Z}{Z} \quad (6)$$

is the fractional difference between the quasiparticle weight $Z = |\langle \psi_0 | c_{\mathbf{k}=0}^{\dagger} | \text{vac} \rangle|^2$ at momentum $\mathbf{k} = 0$ ($|\psi_0\rangle$ denotes the $\mathbf{k} = 0$ groundstate) and the inverse mass renormalization $(m_{||}^0/m_{||})_{t_{\perp}=0}$ at $t_{\perp} = 0$. This relation holds independent of dimension. As a consequence of the momentum dependence of the polaron self-energy, $\delta \neq 0$ is possible⁶. That $\delta > 0$, and thus $A > 0$, results from effective long-range hopping processes induced by electron-phonon-coupling, which reduce $(m_{||}^0/m_{||})_{t_{\perp}=0}$ compared to $1/Z$. In a certain sense, δ measures the deviation from the anti-adiabatic strong-coupling result $m_i/m_i^0 = Z^{-1} = \exp(g^2)$, when $\delta = 0$.

In Fig. 7 we show δ for fixed g^2 as a function of ω_0 . For $\omega_0/t \gg 1$, the ratio δ is close to zero as the anti-adiabatic limit is approached. For $\omega_0 \rightarrow 0$ and fixed g^2 , the ratio δ converges to zero since the weak coupling regime is reached. Decreasing ω_0 or increasing ε_p , the ratio δ , and thus A , can be made very large. For the parameters plotted, A can attain values as large as 27%. Note that A is already large for small coupling $\varepsilon_0/t_{||}$ provided $\omega_0/t_{||}$ is small (see inset in Fig. 7), which implies that the mechanism described here is relevant for realistic materials.

IV. CONCLUSIONS

To sum up, the exact results provided in this work help to clarify the issue of polaron formation in anisotropic 3D

materials, including the 1D and isotropic 3D case. In the extreme adiabatic regime, where large heavy 1D polarons exist for tiny phonon frequencies $\omega_0/t_{||} \ll 0.1$, the scenario of polaron destabilization given by Emin⁸ applies. We present complementary results for the broader regime of small-to-intermediate phonon frequency and small-to-strong coupling strength. In combination with Emin's work at least the most fundamental answers to the Holstein polaron anisotropy problem are thereby given. The regime of very strong coupling or large phonon frequency, where a polaron is always small or its properties do not depend on dimension, deserves no further exploration in that context.

Our findings have two major implications. First, polaron destabilization occurs only in the extreme adiabatic regime, but the concept does not carry over to finite phonon frequencies without significant modifications. Although it is possible to drive a heavy 1D polaron into a light 3D particle by increasing the perpendicular electronic transfer integral, a smooth crossover takes place instead of an instability. In any case, polarons in quasi-1D materials can be described by the 1D Holstein model for small perpendicular transfer integrals. The second implication is that even a local Holstein interaction enhances the anisotropy in electron motion. For small phonon frequencies this enhancement is of significant size already at weak-to-moderate coupling. As a question for future research we mention that the anisotropy enhancement becomes even more important for longer-ranged electron-phonon coupling. We stress that the frequent assumption that the Holstein interaction leads only to isotropic changes of material properties is not true. Experimentally observed anisotropic behaviour provides no indication against a dominating short-range Holstein-like coupling.

Acknowledgments

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¹ H. Fehske and S. A. Trugman, in *Polarons in Advanced Materials*, edited by A. S. Alexandrov (Springer, Dordrecht, 2007), vol. 103 of *Springer Series in Material Sci-*

ences, pp. 393–461.

² V. V. Kabanov and O. Y. Mashtakov, *Phys. Rev. B* **47**, 6060 (1993).

- ³ G. Wellein and H. Fehske, Phys. Rev. B **58**, 6208 (1998).
- ⁴ B. Gerlach and H. Löwen, Rev. Mod. Phys. **63**, 63 (1991).
- ⁵ D. M. Eagles, Phys. Rev. **145**, 645 (1966); D. M. Eagles, Phys. Rev. **181**, 1278 (1969); G. Kalosakas, S. Aubry, and G. P. Tsironis, Phys. Rev. B **58**, 3094 (1998); O. S. Barišić, Phys. Rev. B **73**, 214304 (2006).
- ⁶ L.-C. Ku, S. A. Trugman, and J. Bonča, Phys. Rev. B **65**, 174306 (2002); P. E. Kornilovitch, Phys. Rev. Lett. **81**, 5382 (1998).
- ⁷ M. E. Gershenson, V. Podzorov, A. F. Morpurgo, Rev. Mod. Phys. **78**, 973 (2006).
- ⁸ D. Emin, Phys. Rev. B **33**, 3973 (1986).
- ⁹ D. Ljuić and Z. Ivić, Phys. Rev. B **76**, 052302 (2007).
- ¹⁰ A. H. Romero, D. W. Brown, and K. Lindenberg, Phys. Rev. B **60**, 14080 (1999).
- ¹¹ J. Bonča, S. A. Trugman, and I. Batistić, Phys. Rev. B **60**, 1633 (1999).
- ¹² A. A. Gogolin, Solid State Commun. **50**, 265 (1984).
- ¹³ A. H. Romero, D. W. Brown, and K. Lindenberg, Phys. Lett. A **254**, 287 (1999).
- ¹⁴ A. S. Alexandrov and P. E. Kornilovitch, Phys. Rev. Lett. **82**, 807 (1999); H. Fehske, J. Loos, and G. Wellein, Phys. Rev. B **61**, 8016 (2000).